

# Some Refinements of Large Deviation Tail Probabilities

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## Abstract

We study tail probabilities via some Gaussian approximations. Our results make refinements to large deviation theory. The proof builds on classical results by Bahadur and Rao. Binomial distributions and their tail probabilities are discussed in more detail.

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## 1. Introduction

Let  $X_1, \dots, X_n$  be i.i.d. random variables such that the moment generating function  $\mathbf{E}[\exp(\beta X_1)]$  is finite in a neighborhood of the origin. For fixed  $\mu > \mathbf{E}[X_1]$ , the aim of this paper is to approximate the tail distribution:

$$P_{n,\mu} := \mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\}.$$

If  $\mu$  is close to the mean of  $X_1$  one would usually approximate  $P_{n,\mu}$  by a tail probability of a Gaussian random variable. If  $\mu$  is far from the mean of  $X_1$  the tail probability can be estimated using large deviation theory. According to the Sanov theorem the probability that the deviation from the mean is as large as  $\mu$  is of the order  $\exp(-nD)$  where  $D$  is a constant. Bahadur and Rao [2] improved the estimate of this large deviation probability, and the goal of this paper is to extend the Gaussian tail approximations into situations where one normally uses large deviation techniques.

Let  $\phi$  and  $\Phi$  be the *density function* and the *distribution function* of the standard Gaussian, respectively. Let  $P_0$  denote a probability measure describing the distribution of a random variable  $X$ . Consider the 1-dimensional *exponential family* ( $P_\beta$ ) based on  $P_0$  and given by

$$\frac{dP_\beta}{dP_0}(x) = \frac{\exp(\beta \cdot x)}{\mathcal{Z}(\beta)}$$

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where the denominator is the *moment generating function* (partition function) given by

$$\mathcal{Z}(\beta) = \int \exp(\beta \cdot x) \, dP_0 x = \mathbf{E} [e^{\beta X}].$$

The mean value of  $P_\beta$  is

$$\frac{\mathcal{Z}'(\beta)}{\mathcal{Z}(\beta)} \quad (1)$$

and the range of this function will be denoted  $M$  and will be called *the mean value range* of the exponential family.

For  $\mu$  in interior of  $M$  the *maximum likelihood estimate*  $\hat{\beta}(\mu)$  equals the  $\beta$  such that the mean value of  $P_\beta$  equals  $\mu$ , which in this case is the average of the i.i.d. samples. Put  $P^\mu = P_{\hat{\beta}(\mu)}$ . An equivalent definition of  $\hat{\beta}(\mu)$  can be as the solution of the equation

$$\frac{\mathcal{Z}(\hat{\beta}(\mu))}{e^{\hat{\beta}(\mu)\mu}} = \frac{\mathbf{E} [e^{\hat{\beta}(\mu)X}]}{e^{\hat{\beta}(\mu)\mu}} = \min_{\beta > 0} \frac{\mathbf{E} [e^{\beta X}]}{e^{\beta\mu}} = \min_{\beta > 0} \frac{\mathcal{Z}(\beta)}{e^{\beta\mu}}.$$

Let  $V(\mu)$  denote the variance of  $P^\mu$ .

Information divergence is given by

$$D(P^\mu \| P_0) = \int \ln \left( \frac{dP^\mu}{dP_0}(x) \right) dP^\mu x.$$

We see that

$$D(P^\mu \| P_0) = -\ln \frac{\mathbf{E} [e^{\hat{\beta}(\mu)X}]}{e^{\hat{\beta}(\mu)\mu}} = \hat{\beta}(\mu)\mu - \ln \mathcal{Z}(\hat{\beta}(\mu)). \quad (2)$$

## 2. Approximation of tail distributions for non-lattice valued variables

Introduce the notation

$$\mu^* := \sup\{\mu > \mu_0; D(P^\mu \| P_0) < \infty\} = \sup M.$$

Bahadur and Rao [2] proved a refined version of the large deviation bound, but some aspects of their result dates back to Cramér [4] and part of it was proved by a different method by Blackwell and Hodges [3]. For  $\mu^* > \mu > \mu_0$ , the Sanov theorem implies that

$$-\frac{\ln \mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\}}{n} \rightarrow D(P^\mu \| P_0) \text{ for } n \rightarrow \infty.$$

Bahadur and Rao [2] verified the following improvement of the Sanov theorem

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \frac{\exp(-nD(P^\mu \| P_0))}{(2\pi nV(\mu))^{1/2} \hat{\beta}(\mu)} \left( 1 + O\left(\frac{1}{\sqrt{n}}\right) \right) \text{ for } n \rightarrow \infty \quad (3)$$

for non lattice random variables.

We will write  $D(\mu)$  as short for  $D(P^\mu \| P_0)$ .

**Theorem 1.** For  $\mu^* > \mu > \mu_0$ , one has that

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \Phi \left( -n^{1/2} \left( 2D \left( \mu - \frac{c_\mu}{n} \right) \right)^{1/2} \right) \left( 1 + O \left( \frac{1}{\sqrt{n}} \right) \right) \text{ for } n \rightarrow \infty, \quad (4)$$

where

$$c_\mu = \frac{\ln \frac{(2D(\mu))^{1/2}}{V(\mu)^{1/2} \hat{\beta}(\mu)}}{\hat{\beta}(\mu)}. \quad (5)$$

**Proof.** The  $c_\mu$  defined by (5) satisfies the equation

$$\frac{\left( \frac{2D(\mu)}{V(\mu)} \right)^{1/2}}{\hat{\beta}(\mu) e^{c_\mu \hat{\beta}(\mu)}} = 1. \quad (6)$$

The tail probabilities of the standard Gaussian satisfy

$$\frac{\phi(z)}{z} \left( 1 - \frac{1}{z^2} \right) \leq \Phi(-z) \leq \frac{\phi(z)}{z}$$

for  $z > 0$ , (cf. Feller [5, p. 179]), which implies that

$$\frac{\exp \left( -nD \left( \mu - \frac{c_\mu}{n} \right) \right)}{(2\pi n)^{1/2} \left( 2D \left( \mu - \frac{c_\mu}{n} \right) \right)^{1/2}} = \Phi \left( -n^{1/2} \left( 2D \left( \mu - \frac{c_\mu}{n} \right) \right)^{1/2} \right) \left( 1 + O \left( \frac{1}{n} \right) \right),$$

and so

$$\frac{\exp \left( -nD \left( \mu - \frac{c_\mu}{n} \right) \right)}{(2\pi n)^{1/2} (2D(\mu))^{1/2}} = \Phi \left( -n^{1/2} \left( 2D \left( \mu - \frac{c_\mu}{n} \right) \right)^{1/2} \right) \left( 1 + O \left( \frac{1}{n} \right) \right). \quad (7)$$

Because of (1) and (2), the derivative can be calculated as

$$\frac{d}{d\mu} D(\mu) = \hat{\beta}(\mu),$$

leading to the following Taylor expansion

$$D \left( \mu - \frac{c_\mu}{n} \right) = D(\mu) - \hat{\beta}(\mu) \cdot \frac{c_\mu}{n} + O \left( \frac{1}{n^2} \right).$$

Thus,

$$\begin{aligned} \frac{\exp \left( -nD \left( \mu - \frac{c_\mu}{n} \right) \right)}{(2\pi n)^{1/2} (2D(\mu))^{1/2}} &= \frac{\exp \left( -n \left( D(\mu) - \hat{\beta}(\mu) \cdot \frac{c_\mu}{n} + O \left( \frac{1}{n^2} \right) \right) \right)}{(2\pi n)^{1/2} (2D(\mu))^{1/2}} \\ &= \frac{\exp \left( -nD(\mu) + \hat{\beta}(\mu)c_\mu + O \left( \frac{1}{n} \right) \right)}{(2\pi n)^{1/2} (2D(\mu))^{1/2}} \\ &= \frac{\exp(-nD(\mu)) e^{c_\mu \hat{\beta}(\mu)}}{(2\pi n)^{1/2} (2D(\mu))^{1/2}} \left( 1 + O \left( \frac{1}{n} \right) \right) \end{aligned} \quad (8)$$

According to (3) we also have

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \frac{\exp(-nD(\mu))}{(2\pi nV(\mu))^{1/2} \hat{\beta}(\mu)} \left( 1 + O\left(\frac{1}{\sqrt{n}}\right) \right) \text{ for } n \rightarrow \infty, \quad (9)$$

therefore applying (6), (7), (8) and (9) the proof of Theorem 1 is complete.  $\square$

**Remark 1.** If in the approximation  $c_\mu$  is replaced by any other constant  $c$  then the ratio of the two approximations tends to a number, which is not equal to 1:

$$\begin{aligned} \frac{\exp(-nD(\mu - \frac{c_\mu}{n}))}{\exp(-nD(\mu - \frac{c}{n}))} &= \exp\left(-nD\left(\mu - \frac{c_\mu}{n}\right) + nD\left(\mu - \frac{c}{n}\right)\right) \\ &= \exp\left(\hat{\beta}(\mu) \cdot (c_\mu - c) + O\left(\frac{1}{n}\right)\right) \\ &\approx \exp\left(\hat{\beta}(\mu) \cdot (c_\mu - c)\right) \\ &\neq 1. \end{aligned}$$

**Remark 2.** If  $X_1$  has a density with respect to the Lebesgue measure then Bahadur and Rao [2] proved the stronger result that

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \frac{\exp(-nD(P^\mu \| P_0))}{(2\pi nV(\mu))^{1/2} \hat{\beta}(\mu)} \left( 1 + O\left(\frac{1}{n}\right) \right).$$

Using this result we get the following theorem: If  $X_1$  has a density with respect to the Lebesgue measure then

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \Phi\left(-n^{1/2} \left(2D\left(\mu - \frac{c_\mu}{n}\right)\right)^{1/2}\right) \left( 1 + O\left(\frac{1}{n}\right) \right) \text{ for } n \rightarrow \infty,$$

for any  $\mu^* > \mu > \mu_0$ .

### 3. Results for lattice valued variables

Now assume that  $X_1, X_2, \dots$  is a sequence of i.i.d. random variables with values in a lattice of the type  $\{kd + \delta \mid k \in \mathbb{Z}\}$ . For such a sequence Bahadur and Rao [2] proved that

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \frac{\exp(-nD(P^\mu \| P_0))}{(2\pi nV(\mu))^{1/2} \frac{1 - \exp(-d\hat{\beta}(\mu))}{d}} \left( 1 + O\left(\frac{1}{n}\right) \right) \quad (10)$$

for any  $n$  such that  $\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i = \mu \right\} > 0$ . We note that the result (3) for non-lattice variables can be considered as a limiting version of (10) for small  $d > 0$  because

$$\frac{1 - \exp(-d\beta)}{d} \rightarrow \beta \text{ for } d \rightarrow 0.$$

**Theorem 2.** Assume that  $X_1$  has values in the lattice  $\{kd + \delta \mid k \in \mathbb{Z}\}$  and that  $\mu^* > \mu > \mu_0$ . Then for any  $n$  such that  $\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i = \mu \right\} > 0$  one has

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \Phi \left( -n^{1/2} \left( 2D \left( \mu - \frac{c_\mu}{n} \right) \right)^{1/2} \right) \left( 1 + O \left( \frac{1}{n} \right) \right) \text{ for } n \rightarrow \infty,$$

where

$$c_\mu = \frac{\ln \frac{(2D(\mu))^{1/2}}{V(\mu)^{1/2} \frac{1 - \exp(-d\hat{\beta}(\mu))}{d}}}{\hat{\beta}(\mu)}.$$

**Proof.** If  $X_1$  is lattice valued then the proof of Theorem 1 can be modified by replacing  $\hat{\beta}(\mu)$  by  $\frac{1 - \exp(-d\hat{\beta}(\mu))}{d}$  at the appropriate places throughout the proof. There is no modification in the use of a Taylor expansion.  $\square$

We now turn to the special case, where  $X_1, \dots, X_n$  are i.i.d. Bernoulli random variables with

$$X_i = \begin{cases} 1 & \text{with probability } p, \\ 0 & \text{with probability } 1 - p. \end{cases}$$

In this case  $d = 1$ , and  $\sum_{i=1}^n X_i$  is a binomial  $(n, p)$  random variable. For various refinements of (10), see Bahadur [1], Littlewood [8] and McKay [9].

**Corollary 1.** Put

$$\mu_n := \lceil n\mu \rceil / n.$$

Then for  $1 > \mu > p$  one has that

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \Phi \left( -n^{1/2} \left( 2D \left( \mu_n - \frac{c_{\mu_n}}{n} \right) \right)^{1/2} \right) \left( 1 + O \left( \frac{1}{n} \right) \right) \text{ for } n \rightarrow \infty,$$

where

$$D(\mu) = D(\mu \| p) = \mu \ln \frac{\mu}{p} + (1 - \mu) \ln \frac{1 - \mu}{1 - p}$$

and

$$c_\mu = \frac{1}{2} + \frac{\ln \left( \frac{2D(\mu \| p)}{(\mu - p)^2} p(1 - p) \right)}{2 \ln \frac{\mu(1 - p)}{p(1 - \mu)}}.$$

**Proof.** Because of the definition of  $\mu_n$ ,

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu_n \right\},$$

and the condition  $\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i = \mu_n \right\} > 0$  is satisfied, and so Theorem 2 implies that

$$\mathbf{P} \left\{ \frac{1}{n} \sum_{i=1}^n X_i \geq \mu \right\} = \Phi \left( -n^{1/2} \left( 2D \left( \mu_n - \frac{c_{\mu_n}}{n} \right) \right)^{1/2} \right) \left( 1 + O \left( \frac{1}{n} \right) \right) \text{ for } n \rightarrow \infty.$$

We have to evaluate  $c_\mu$ . The distribution  $P_\beta$  has

$$P_\beta(X_i = 1) = \frac{pe^\beta}{1 - p + pe^\beta}$$

which is also the mean of  $P_\beta$ . The equation

$$\mu = \frac{pe^\beta}{1 - p + pe^\beta}$$

is equivalent to

$$e^\beta = \frac{\mu(1-p)}{p(1-\mu)}$$

implying that

$$\frac{1 - e^{-d\beta}}{d} = 1 - e^{-\beta} = 1 - \frac{p(1-\mu)}{\mu(1-p)} = \frac{\mu - p}{\mu(1-p)}.$$

The variance function is

$$V(\mu) = \mu(1-\mu).$$

Thus, we have

$$\begin{aligned} c_\mu &= \frac{\ln \left( \left( \frac{2D(\mu||p)}{V(\mu)} \right)^{1/2} \frac{1}{1 - e^{-\hat{\beta}(\mu)}} \right)}{\hat{\beta}(\mu)} \\ &= \frac{\ln \left( \left( \frac{2D(\mu||p)}{\mu(1-\mu)} \right)^{1/2} \frac{\mu(1-p)}{\mu-p} \right)}{\ln \frac{\mu(1-p)}{p(1-\mu)}} \\ &= \frac{1}{2} + \frac{\ln \left( \frac{2D(\mu||p)}{(\mu-p)^2} p(1-p) \right)}{2 \ln \frac{\mu(1-p)}{p(1-\mu)}}. \end{aligned}$$

□

**Remark 3.** For  $p = 1/2$ ,  $0.5 < c_\mu < 0.534$  and Table 1 shows some numerical values for  $c_\mu \approx 0.5 + (\mu - 0.5)/12$ .

$\mu$	0.6	0.65	0.7	0.75	0.8	0.85	0.9
$c_\mu$	0.508	0.512	0.516	0.520	0.524	0.528	0.532

Table 1: Numerical values

#### 4. Discussion

As discussed by Reiczigel, Rejtő and Tusnády [10] and by Harremoës and Tusnády [6] there are some strong indications that these asymptotic results can be strengthened

to sharp inequalities. Such sharp inequalities would imply the present asymptotic results as corollaries. We hope that the asymptotics presented here can help in proving the conjectured sharp inequalities. Related sharp inequalities have been discussed by Leon and Perron [7] and Talagrand [11]. Numerical experiments have also shown that our tail estimates are useful even for small values of  $n$ .

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